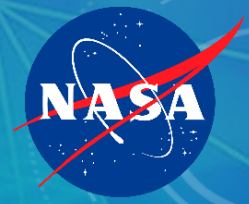
National Aeronautics and Space Administration



Recent progress in spin defect metrology at NASA Glenn's Quantum Sensing and Spin Physics (Q-SASP) lab

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San Francisco, CA
1/27/24

What is Quantum Sensing and Why?

What is Quantum Sensing used for?

Because quantum sensing measures activity in the physical world using atomic properties, the significantly more accurate data it provides can make future versions of technologies that already exist today function better, collecting and using better information to yield better results.

How does Quantum Sensing extract data at the atomic level?

Quantum Sensors use what are called “quantum resources” to measure changes in atoms with a higher degree of precision than classical measurements can. Quantum resources are physical qualities that don’t exist in classical physics, including entanglement, superposition, discrete states, and coherence. For example, quantum optics typically relies on measurements using various aspects of light, or photons, but quantum sensors can also be made from other mediums, such as atoms in free space and point defects in solid-state devices.

Outline

Objective: Explore spin-dependent interactions in SiC solid-state devices

I. Electrically detect the magnetic resonance signal at a near zero magnetic field by measuring the spin dependent current

II. Understanding the properties of the defects in SiC by computational simulations

III. Utilize near zero field magnetic resonance technique to determine the zero-field spitting parameters of defects in SiC diodes

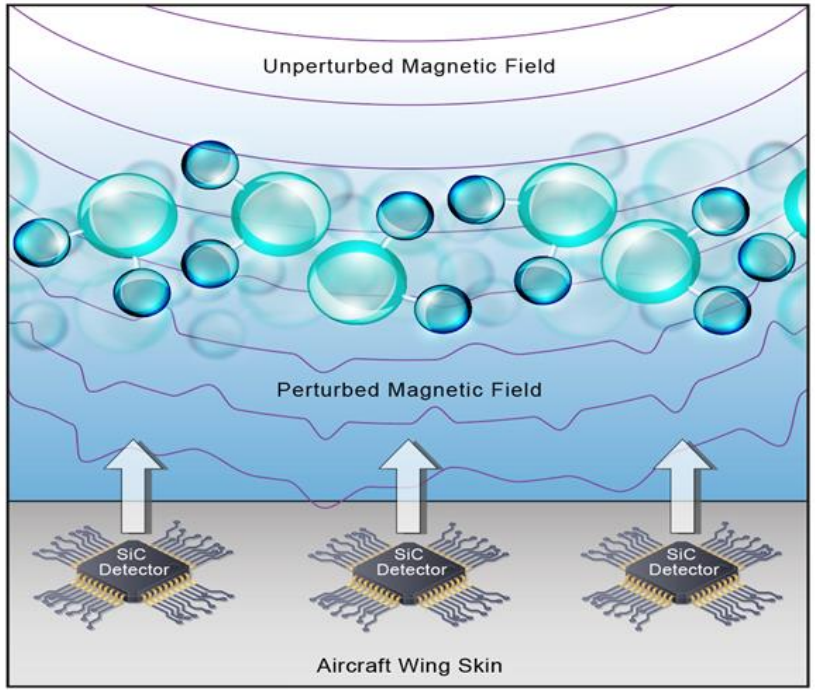
IV. Evaluate performance of various non-metal implant in SiC pin diode

NASA Space Communications and Navigation (SCaN)

Contribution: Build self-calibrating spin defect quantum magnetometer sensor network (near-term) and a solid-state spin-based quantum memory and/or repeater for future communication systems (far-term)

Quantum Sensors and Instruments

Icing Mitigation

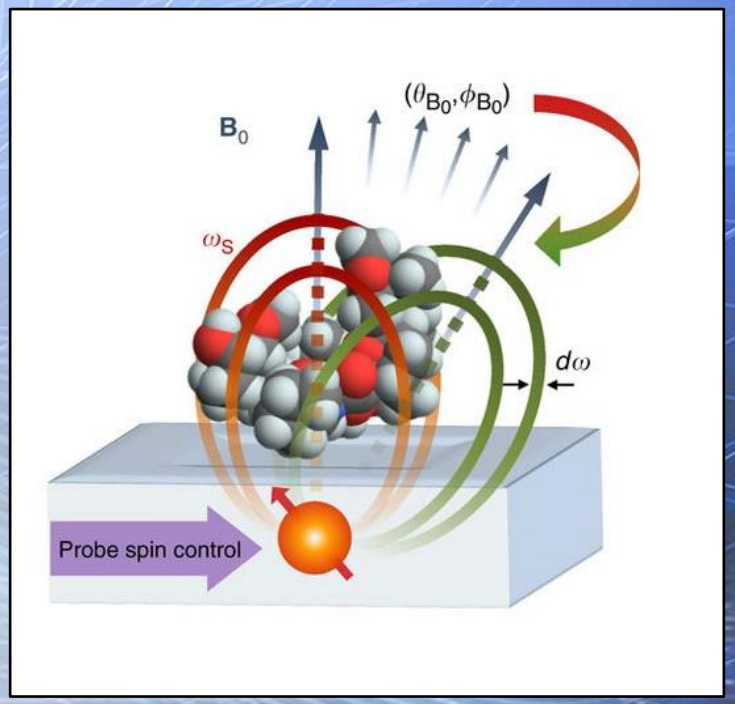


(Ice polytypes on aircraft wing)

Nanoscale Chemical Analysis for planetary missions

Credit: EESA

Nanoscale MRI for space application



Credit: Perunicic et al., *Nature*

EDMR vs EPR

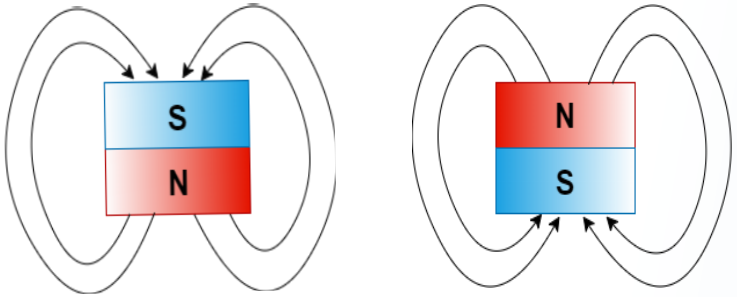
- Increased sensitivity allowing for study of smaller structures > identify centers involved in carrier generation and recombination process
- Electron paramagnetic resonance (EPR) requires 10^{10} ~ 10^{11} defects
- Electrically Detected Magnetic Resonance (EDMR) achieves the same sensitivity with only 10^{2} ~ 10^{3} defects

Credit: Nanalytics

Credit: NASA JPL

Electron Paramagnetic Resonance (EPR)

A B



$m_s = +\frac{1}{2}$ $m_s = -\frac{1}{2}$

Magnetic moment of e^- :

$$\mu_s = -g_e \mu_\beta \hat{\boldsymbol{S}}$$

Spin Hamiltonian:

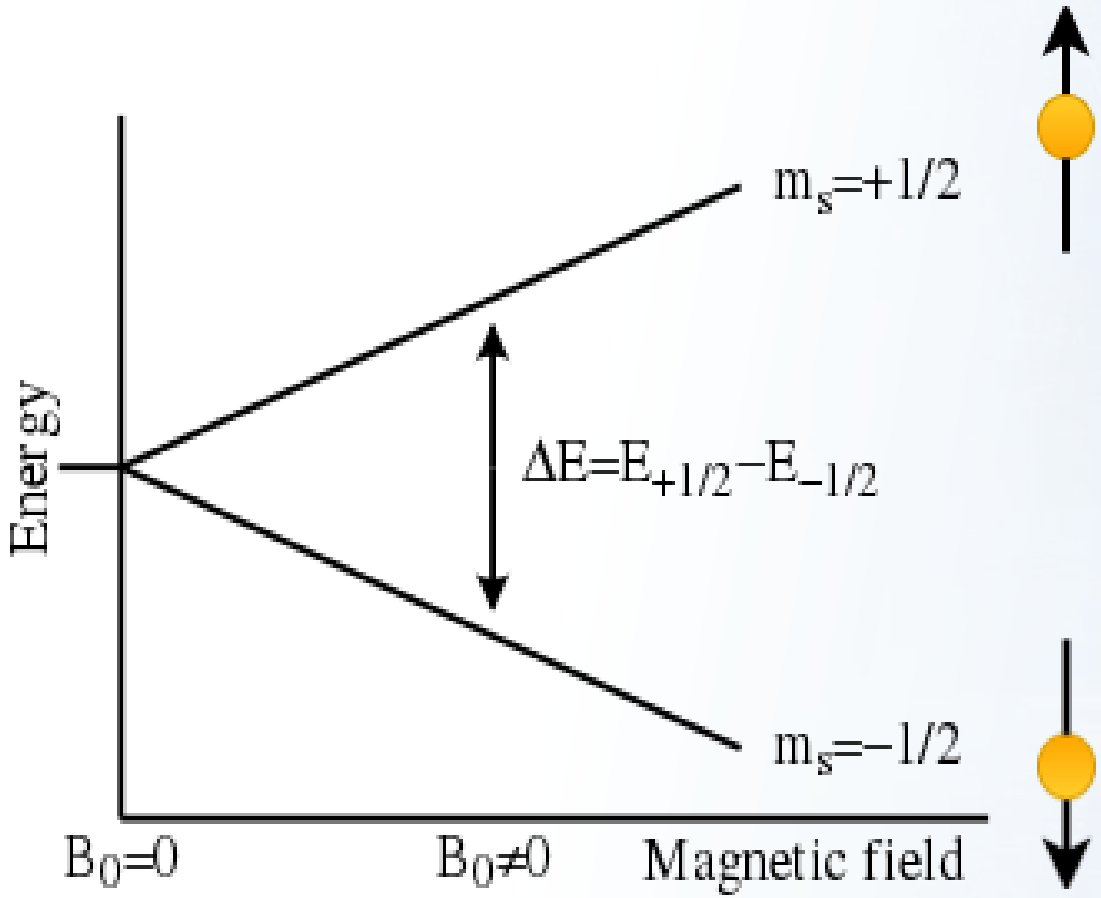
$$\mathcal{H} = g_e \mu_\beta \hat{\boldsymbol{S}} \cdot \boldsymbol{B}$$

$$E_{m_s} = +g_e \mu_\beta B_0 m_s$$

$$E_{\pm 1/2} = \pm \frac{1}{2} g_e \mu_\beta B_0$$

$\hat{\boldsymbol{S}} = total\ spin\ operator$
$\boldsymbol{B} = External\ magnetic\ field\ vector$
$g_e = Landé\ g\ value$
$\mu_\beta = Bohr\ Magneton = \frac{e\hbar}{2m_e}$
$h = Planck's\ constant$
$\boldsymbol{v} = frequency\ of\ oscillating\ mag.field$

Electron Paramagnetic Resonance (EPR)



$$\Delta E = h\nu = g_e \mu_\beta B_0$$

$$E_{m_s} = +g_e \mu_\beta B_0 m_s$$

$$E_{\pm 1/2} = \pm \frac{1}{2} g_e \mu_\beta B_0$$

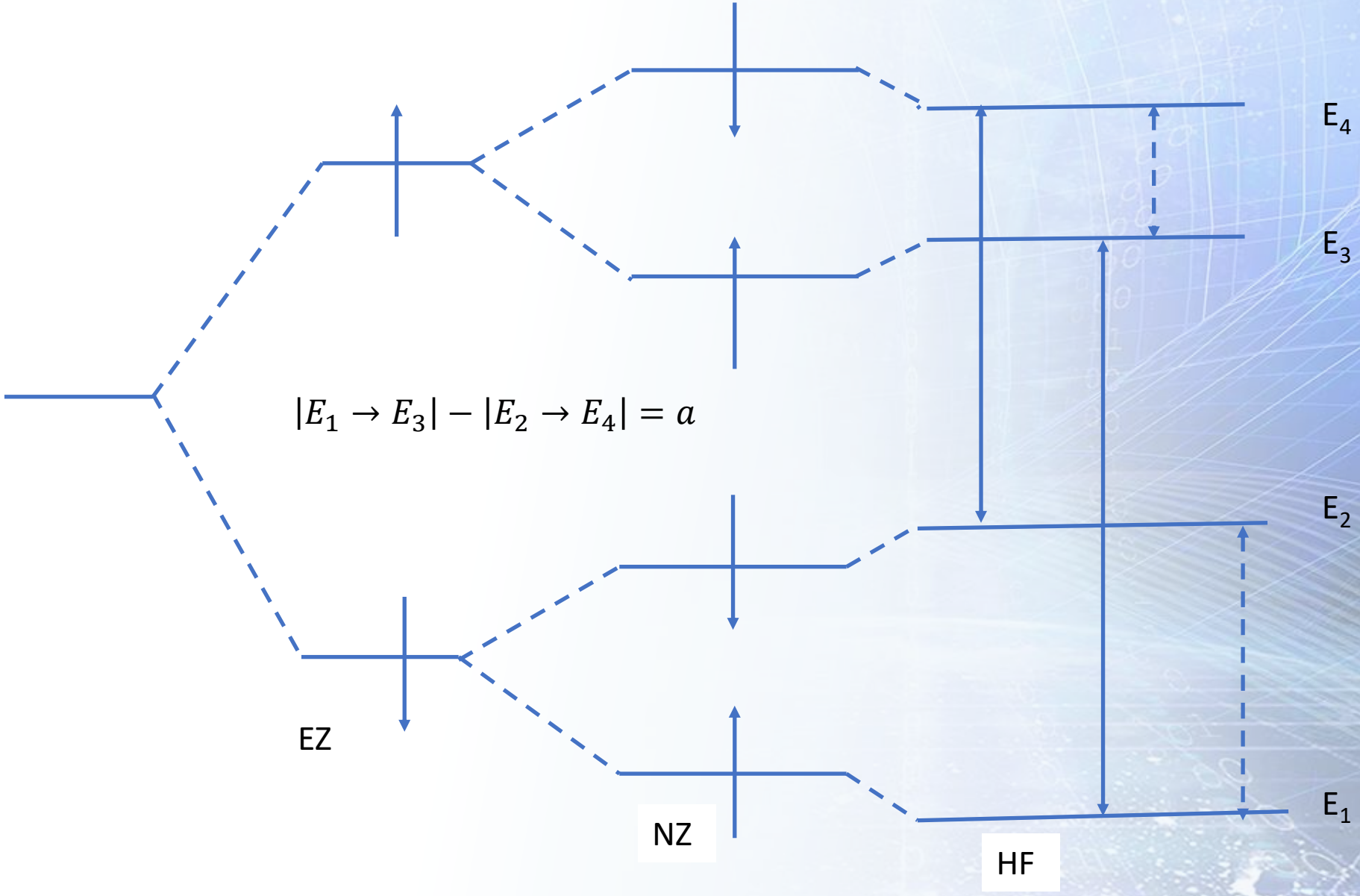
Nuclear Spin and Hyperfine Interactions

- The presence of nuclei with magnetic spin *(I)* adds further interaction to the electron spin system

- These interactions give rise to additional terms to the electron Zeeman Hamiltonian which create perturbations electron spin energies (E)

$$E = g\mu_\beta B m_s - g_N \mu_N B m_I + a m_S m_I$$

Nuclear Spin and Hyperfine Interactions



Electron Paramagnetic Resonance Theory (EDMR)

For a spin-pair system consisting of two electron spins ($S_a = S_b = 1/2$), the time-independent spin-pair Hamiltonian is given by

$$\widehat{\mathcal{H}}_0 = \widehat{\mathcal{H}}_Z + \widehat{\mathcal{H}}_{HF} + \widehat{\mathcal{H}}_{EX} + \widehat{\mathcal{H}}_{DD,ee}$$

$$\mathcal{H} = g\mu_\beta \boldsymbol{B} \cdot (\boldsymbol{S}_1 + \boldsymbol{S}_2) + \sum_{i}^{2} \sum_{j}^{N} \boldsymbol{S}_i \cdot \boldsymbol{A}_{i,j} \cdot \boldsymbol{I}_j - \boldsymbol{J_0 S}_1 \cdot \boldsymbol{S}_2 + \boldsymbol{S}_1 \cdot \boldsymbol{D} \cdot \boldsymbol{S}_2$$

(Zeeman Interaction)

(Nuclear Hyperfine Interaction)

Electron Exchange Interaction)

Electron Dipole-Dipole Coupling Interaction)

Electron Paramagnetic Resonance Theory (EDMR)

For the sake of simplicity, first ignore the hyperfine interactions and spin-spin interactions. the Hamiltonian can be rewritten as:

$$\mathcal{H} = g\mu_\beta \boldsymbol{B} \cdot \boldsymbol{S}$$

where $\boldsymbol{S}(= \boldsymbol{S}_1 + \boldsymbol{S}_2)$ is the total spin operator. By applying the Hamiltonian on the spin wave function $|s, m_s\rangle$, one can get

$$\mathcal{H}|s, m_s\rangle = g\mu_\beta\left(\hat{B}_x + \hat{B}_y + \hat{B}_z\right) \cdot \left(\hat{S}_x + \hat{S}_y + \hat{S}_z\right)|s, m_s\rangle = g\mu_\beta B_0 \hat{S}_z|s, m_s\rangle = m_s g\mu_\beta B_0|s, m_s\rangle$$

where m_s denotes the sum of m_{s1} and m_{s2}. The singlet and triplet energy states are:

$$\mathcal{H}|0,0\rangle = 0$$

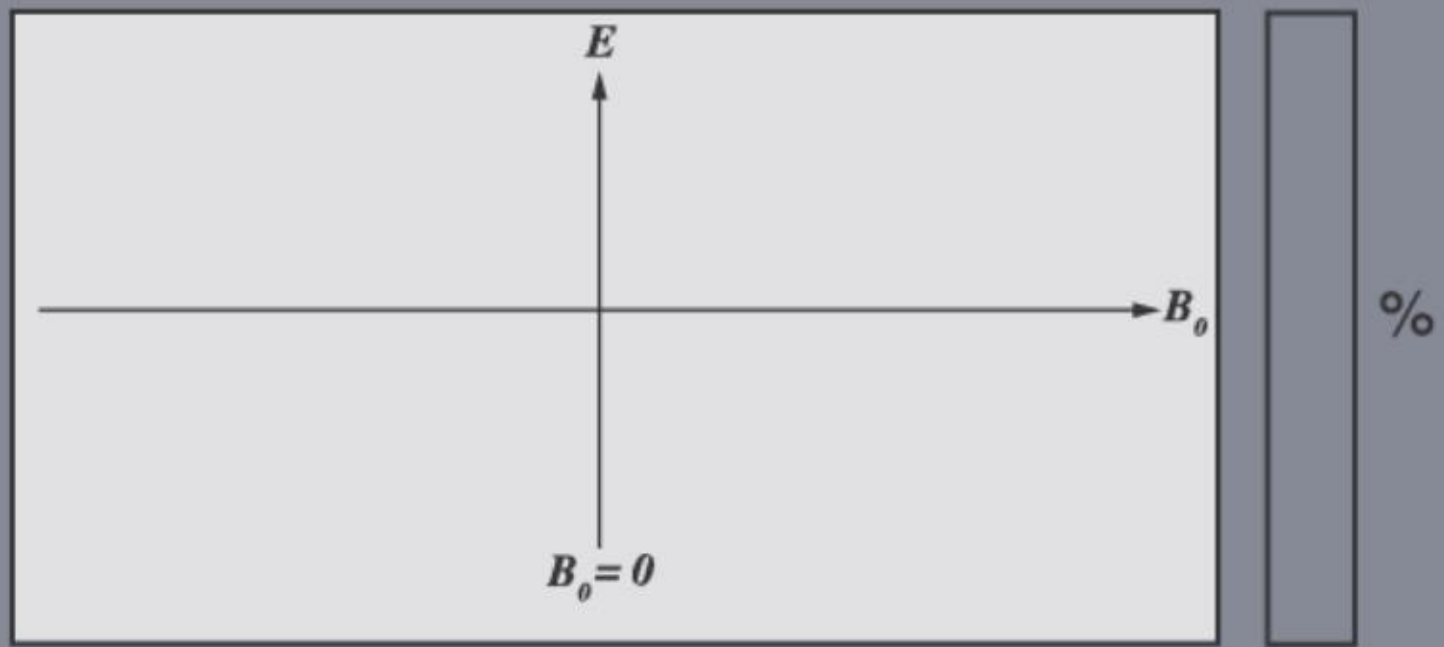
$$\mathcal{H}|1,+1\rangle = g\mu_\beta B_0|1,+1\rangle$$

$$\mathcal{H}|1,0\rangle = 0$$

$$\mathcal{H}|1,-1\rangle = -g\mu_\beta B_0|1,-1\rangle$$

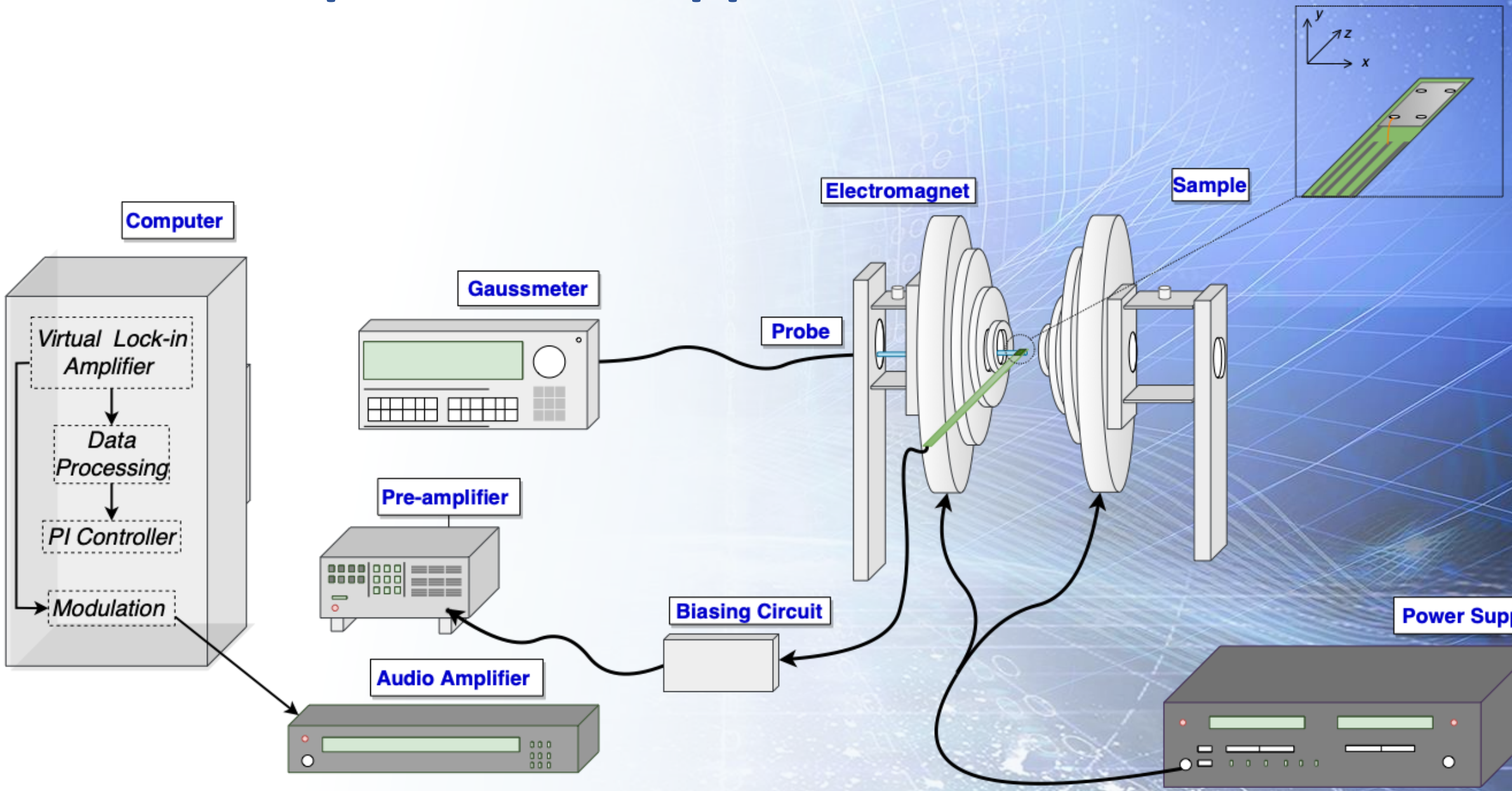
Now, the important point is that at a zero magnetic field, the singlet and triplet states are all degenerate with zero energy. As a result, the triplet states can *mix* with the singlet states. This singlet-triplet mixing allows the triplet states to transition into singlet states without being applied electromagnetic radiation, because, at a zero magnetic field, these two states are energetically accessible.

Electron Zeeman Interaction Only



Generation Recombination

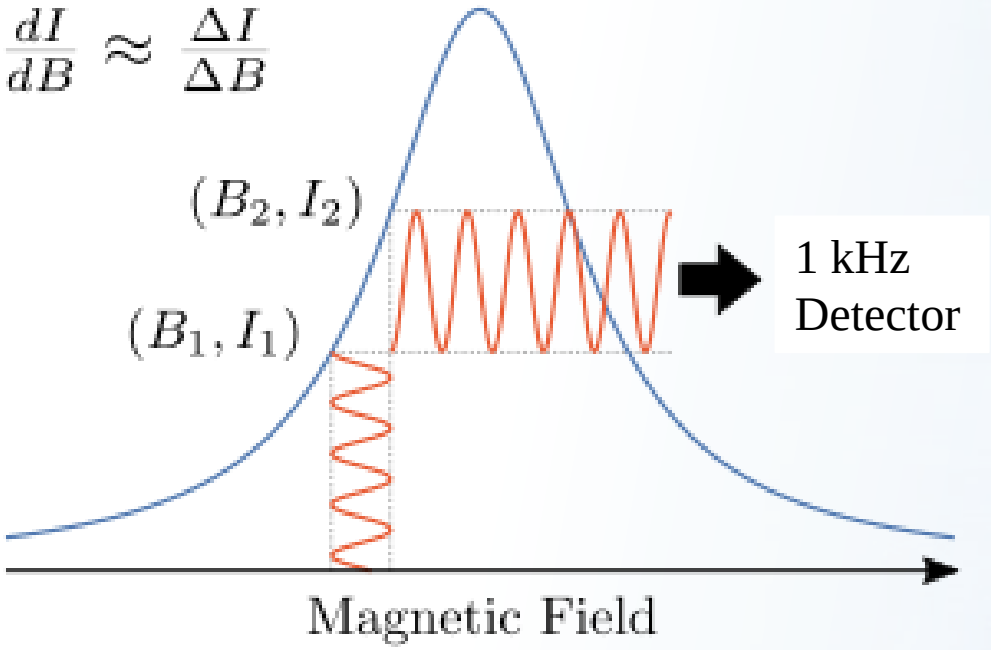
Experimental Apparatus

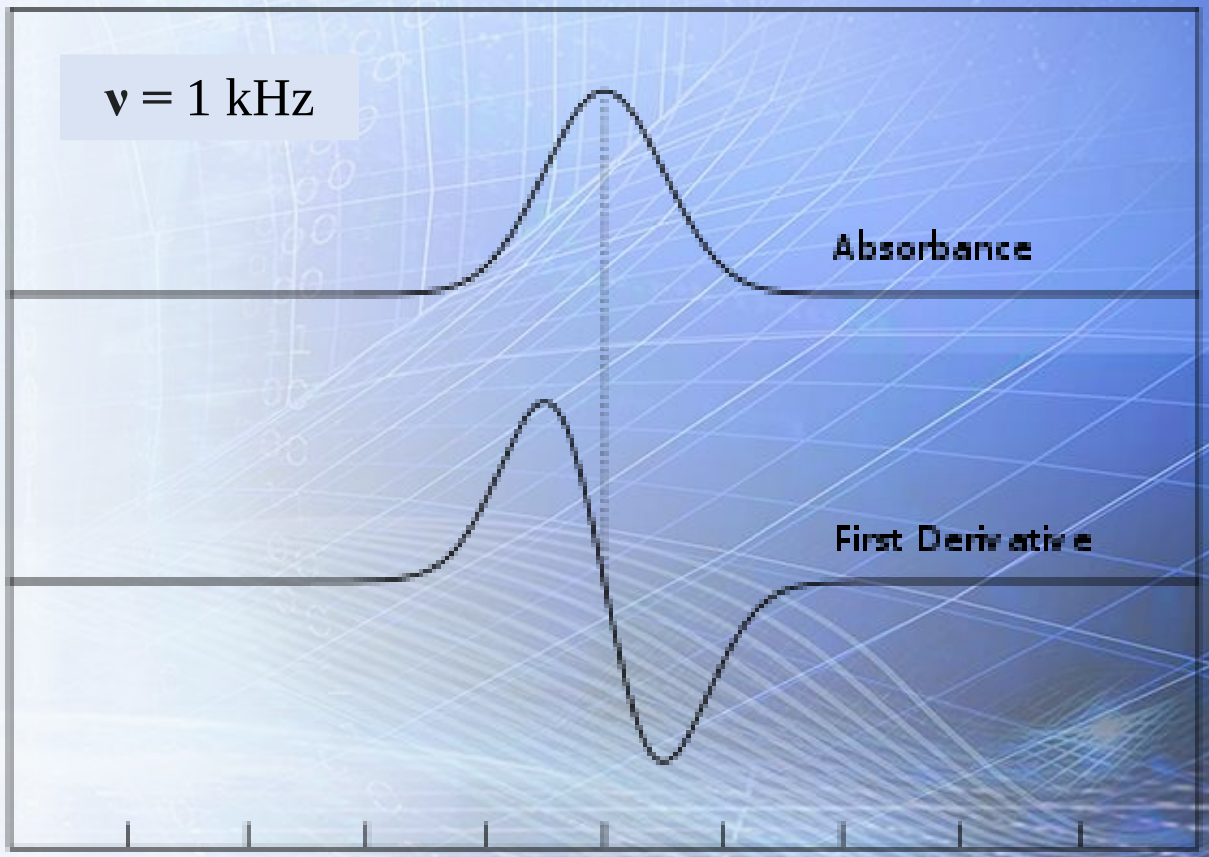


Noise Reduction Method

Magnetic Field Modulation

- Apply small oscillating field
- High S/N ratio
- Derivative Form Signal





Formation Energy

A primary interest is to find the defect formation energy — the energetic cost to create a defect in a bulk material. The defect formation energy E^f of a defect X in charge state q can be computed as follows [1]-[4]:

$$E^f[X^q] = E_{\text{tot}}[X^q] - E_{\text{tot}}[\text{bulk}] - \sum_i n_i \mu_i + qE_F + E_{\text{corr}}.$$

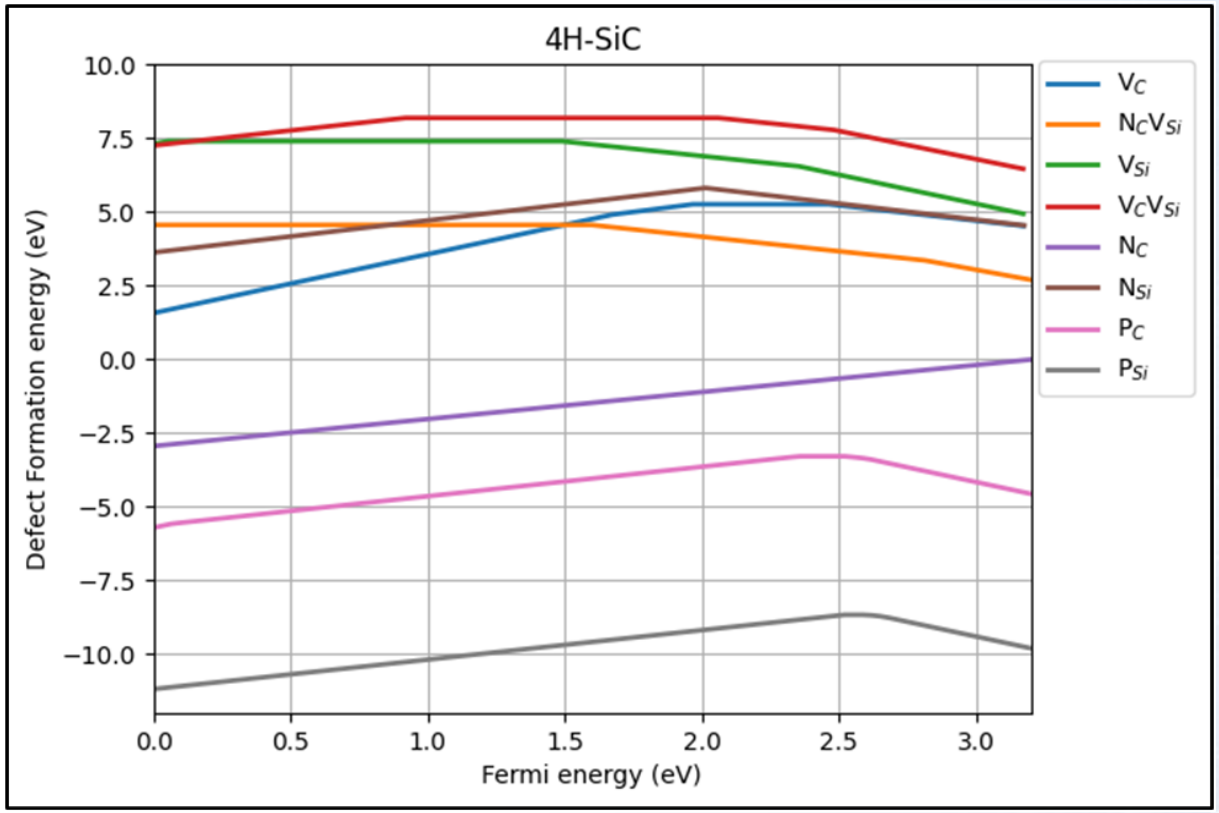
$E_{\text{tot}}[X^q]$ is the total energy of the host crystal *with* the defect, and $E_{\text{tot}}[\text{bulk}]$ is the total energy of the same cell of the crystal *without* the defect. Both can be derived from the DFT calculation. The third term $\sum_i n_i \mu_i$ is a summation of the atomic chemical potentials (the energy cost of an atom being added or removed from the bulk undefective cell.

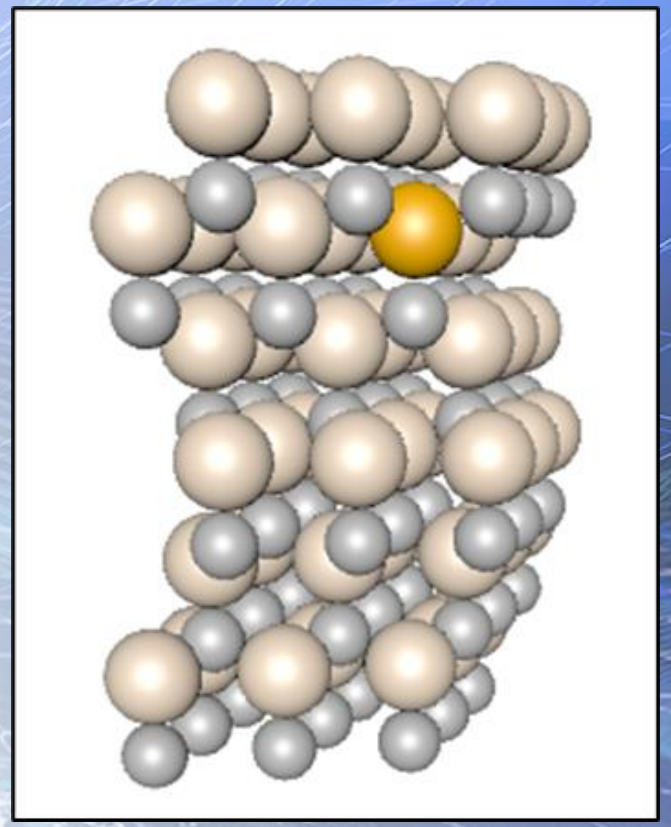
Formation Energy

Formation energy of various types of defects in 4H-SiC and 6H-SiC

Computed with a Density Functional Theory (DFT) calculation software (GPAW)

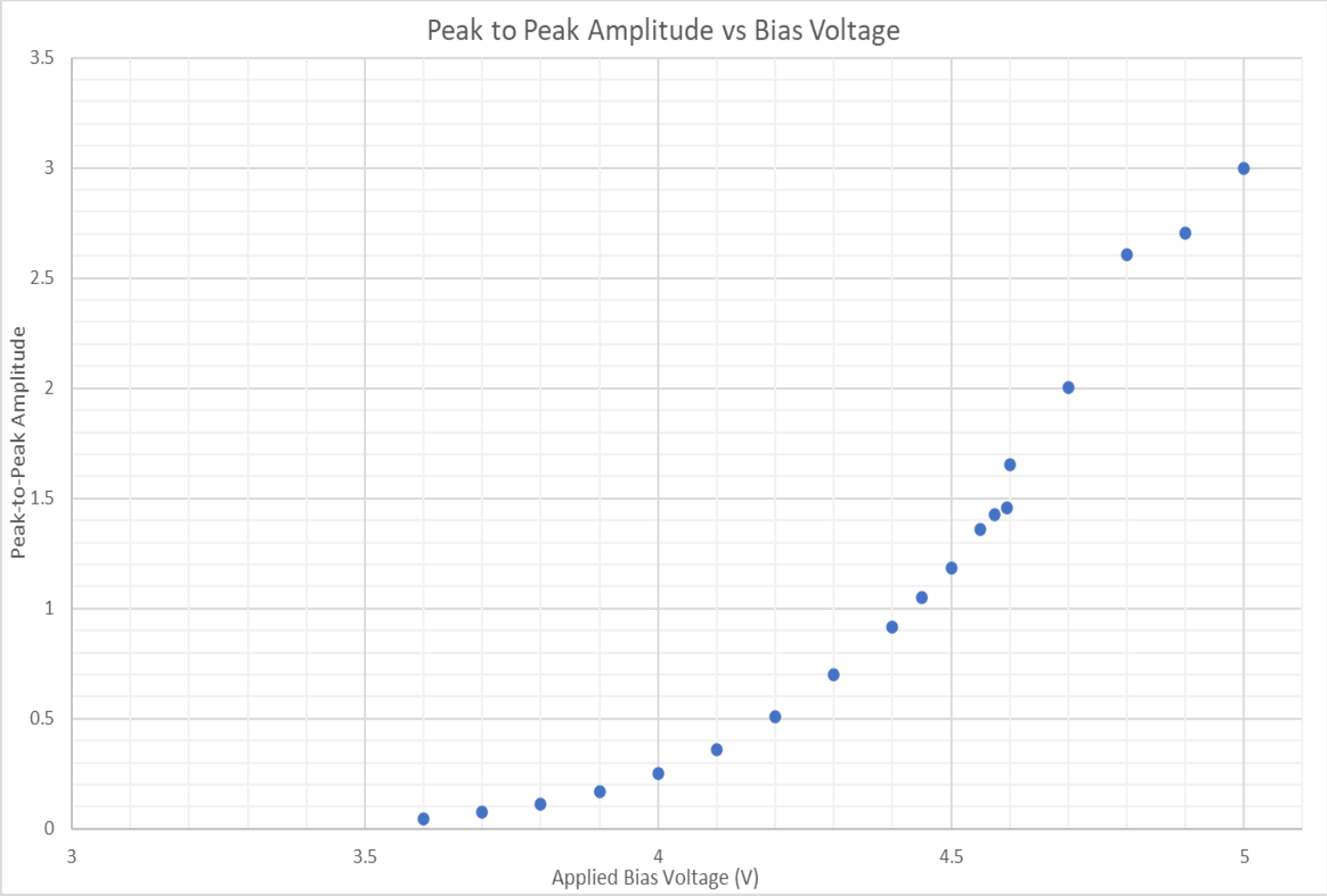
$$E^f[X^q] = E_{\text{tot}}[X^q] - E_{\text{tot}}[\text{bulk}] - \sum_i n_i \mu_i + qE_F + E_{\text{corr}}$$





Substitution of Si by P (P_{Si})

Demonstration of Spin Dependent Recombination



Amplitude peak-to-peak vs applied voltage

Since the device is a well-behaved and well-understood pn-junction, this feature can be described by spin dependent recombination as the primary mechanism for the relation of peak-to-peak amplitude and applied voltage

Dipole-Dipole Interaction Theory

$$\mathcal{H} = \boldsymbol{S}_1 \cdot \boldsymbol{D} \cdot \boldsymbol{S}_2$$

where

$$\boldsymbol{D} = \begin{bmatrix} D_{xx} & D_{yx} & D_{zx} \\ D_{xy} & D_{yy} & D_{zy} \\ D_{xz} & D_{yz} & D_{zz} \end{bmatrix}$$

$$D_{ij} = \frac{\mu_0}{4\pi} g^2 \mu_\beta^2 \left\langle \frac{\delta_{ij}}{\boldsymbol{r}^3} - 3\frac{ij}{\boldsymbol{r}^5} \right\rangle$$

If the principle axes are known, then the dipolar coupling matrix can be written as a diagonal matrix,

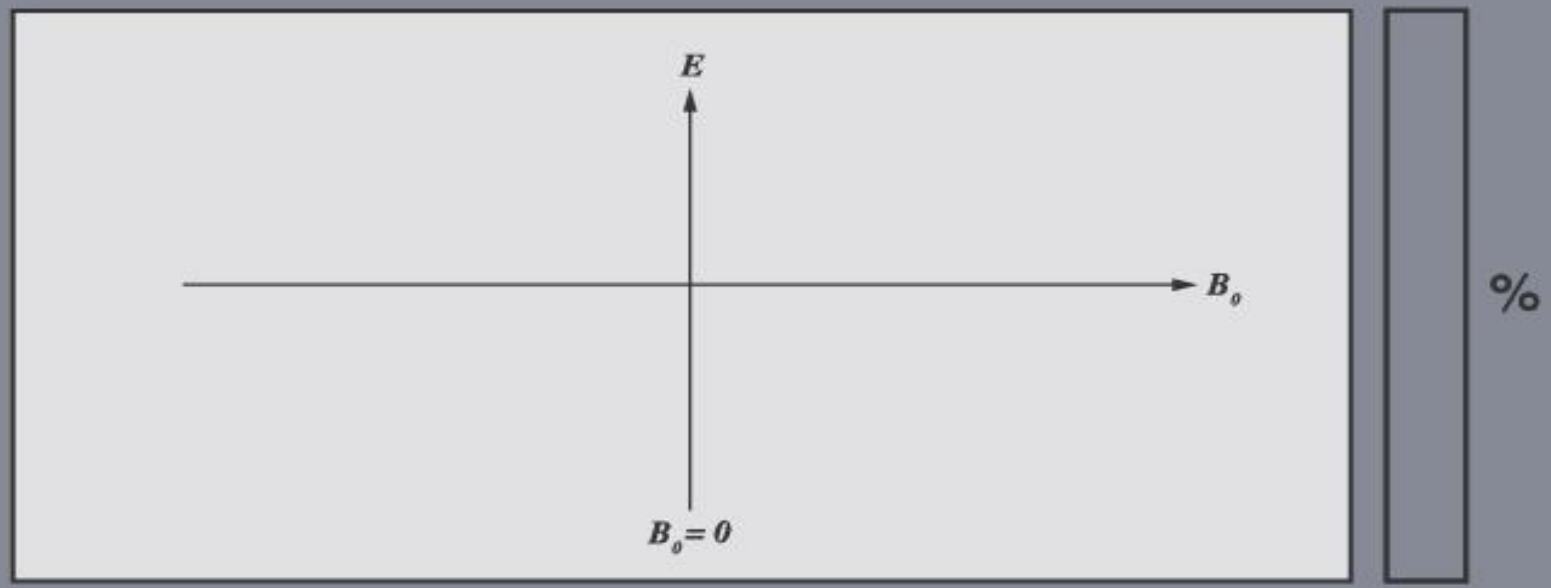
$$\boldsymbol{D} = \begin{bmatrix} D_{xx} & 0 & 0 \\ 0 & D_{yy} & 0 \\ 0 & 0 & D_{zz} \end{bmatrix}$$

It is common to write the diagonal components in terms of the two independent parameters,

$$D = \frac{3}{2} D_{zz}$$

$$E = \frac{1}{2}\left(D_{xx} - D_{yy}\right)$$

Electron Zeeman and Dipole-Dipole Interaction Only



Generation Recombination

Exchange Interaction Theory

The exchange interaction also causes the split peak at a zero field, but the mechanism is different. Assuming an isotropic interaction, the Hamiltonian is given by

$$\mathcal{H} = -J_0 \boldsymbol{S}_1 \cdot \boldsymbol{S}_2$$

where J_0 denotes the exchange parameter. In general, the magnitude of J_0 is dependent on the Coulombic interactions between two electrons, electron spacing, and wave function overlap. In the absence of a magnetic field, the triplet states are degenerate and are separated in energy from the singlet state by a factor of J_0.

$\mathcal{H}|0,0\rangle = J_0 \frac{3}{4}|0,0\rangle$ (Singlet state)

$\mathcal{H}|0,0\rangle = -J_0 \frac{1}{4}|1, m_s\rangle$ (Triplet states)

When placed in a magnetic field, the Hamiltonian becomes $\mathcal{H} = g\mu_\beta \boldsymbol{B} \cdot \boldsymbol{S} - J_0 \boldsymbol{S}_1 \cdot \boldsymbol{S}_2$ so that the energy of each state is

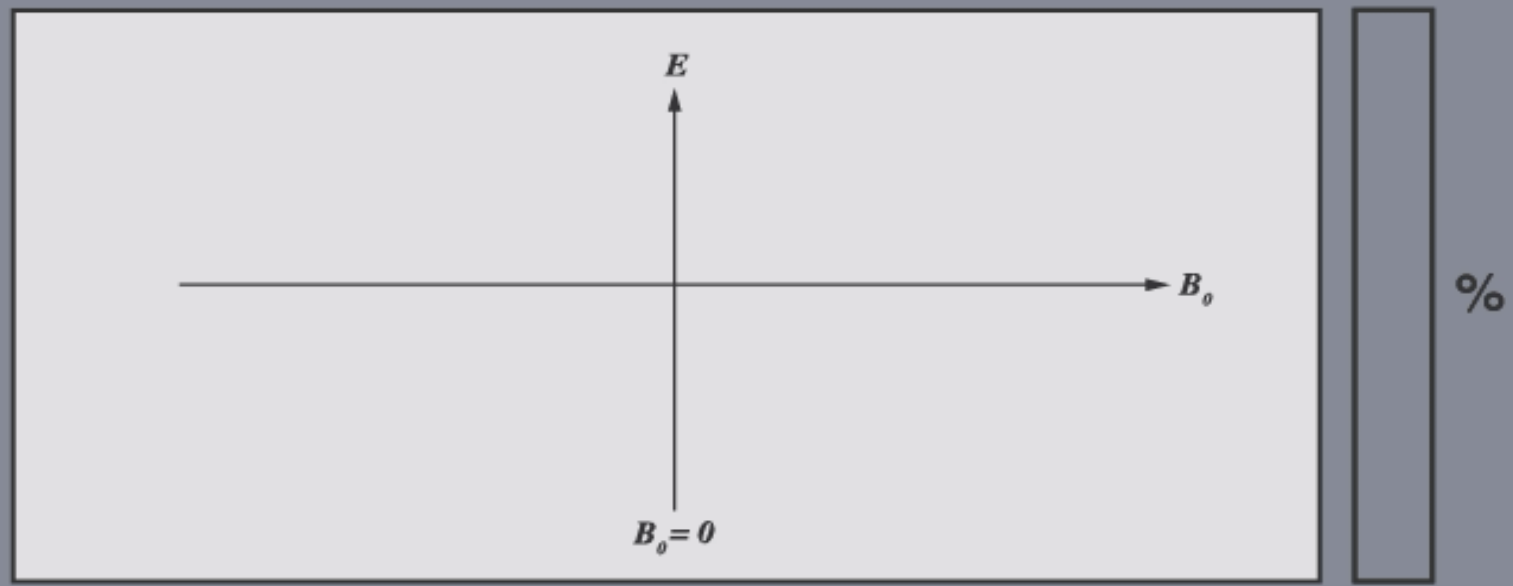
$$\mathcal{H}|0,0\rangle = J_0 \frac{3}{4}|0,0\rangle$$

$$\mathcal{H}|1,+1\rangle = (g\mu_\beta B_0 - J_0 \frac{1}{4})|1,+1\rangle$$

$$\mathcal{H}|1,0\rangle = -J_0 \frac{1}{4}|1,0\rangle$$

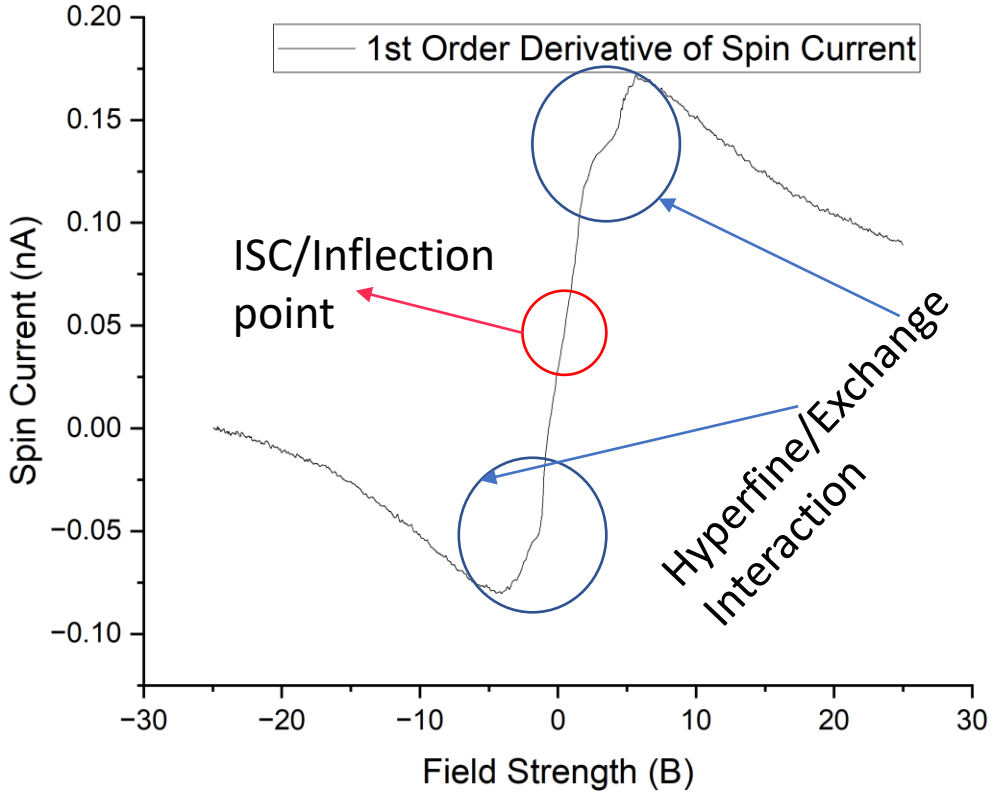
$$\mathcal{H}|0,0\rangle = (-g\mu_\beta B_0 - J_0 \frac{1}{4})|0,0\rangle$$

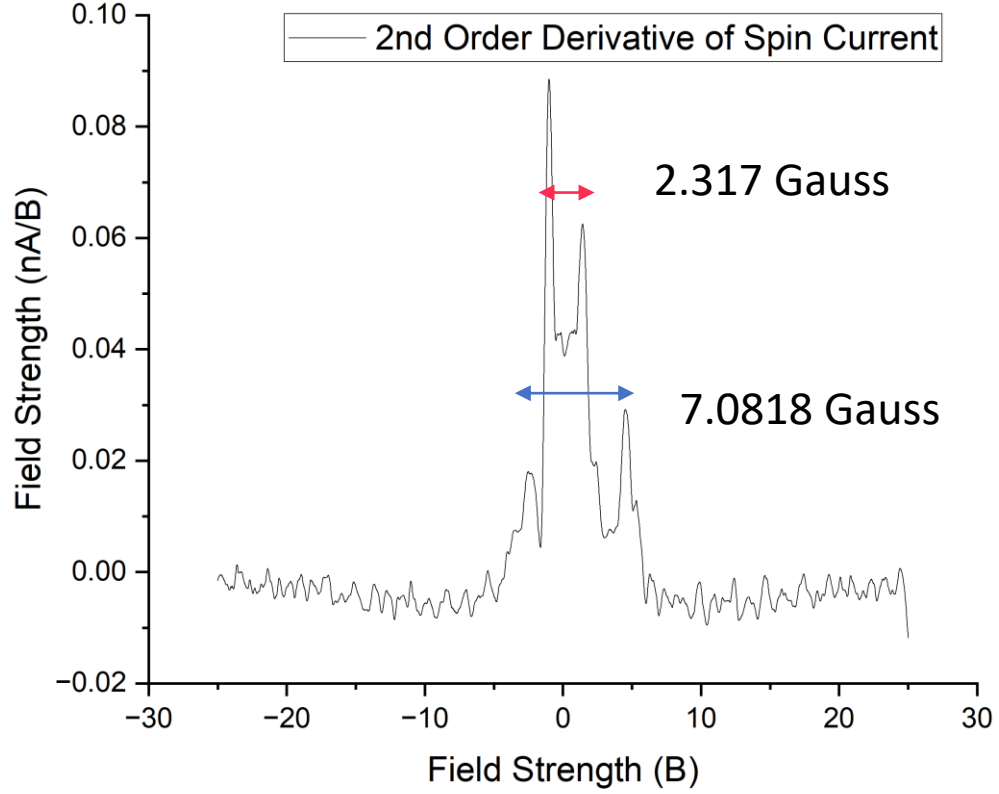
Electron Zeeman and Exchange Interaction Only



Generation Recombination

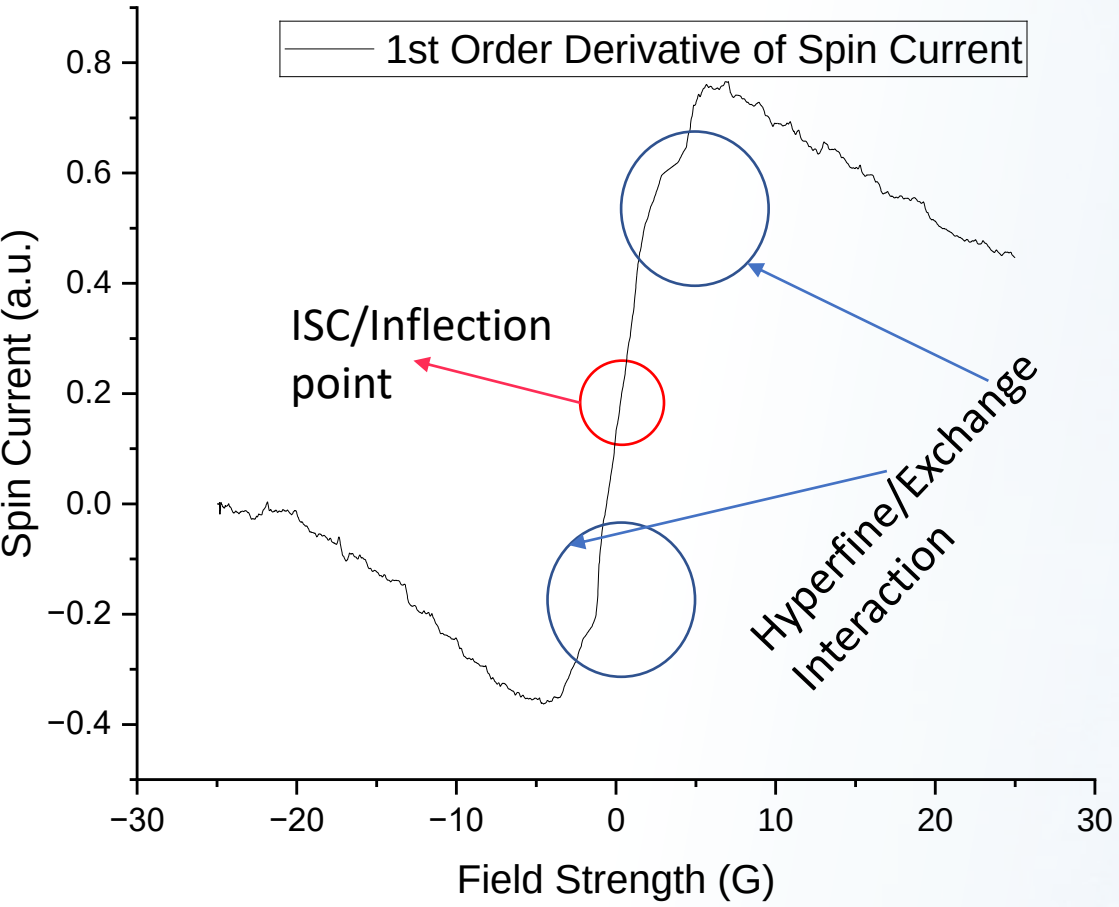
EDMR Spectra (4.0 Volt Bias)

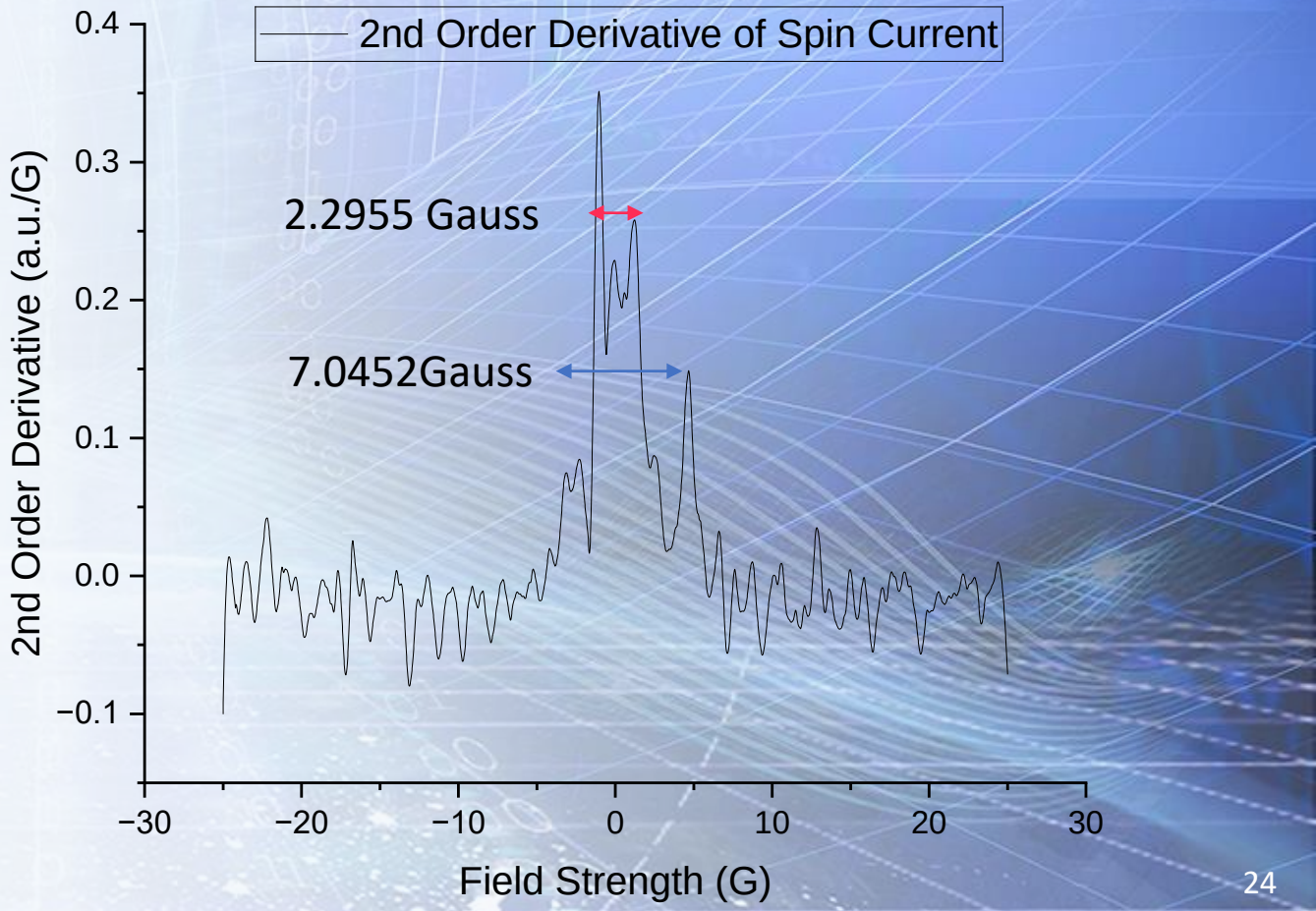




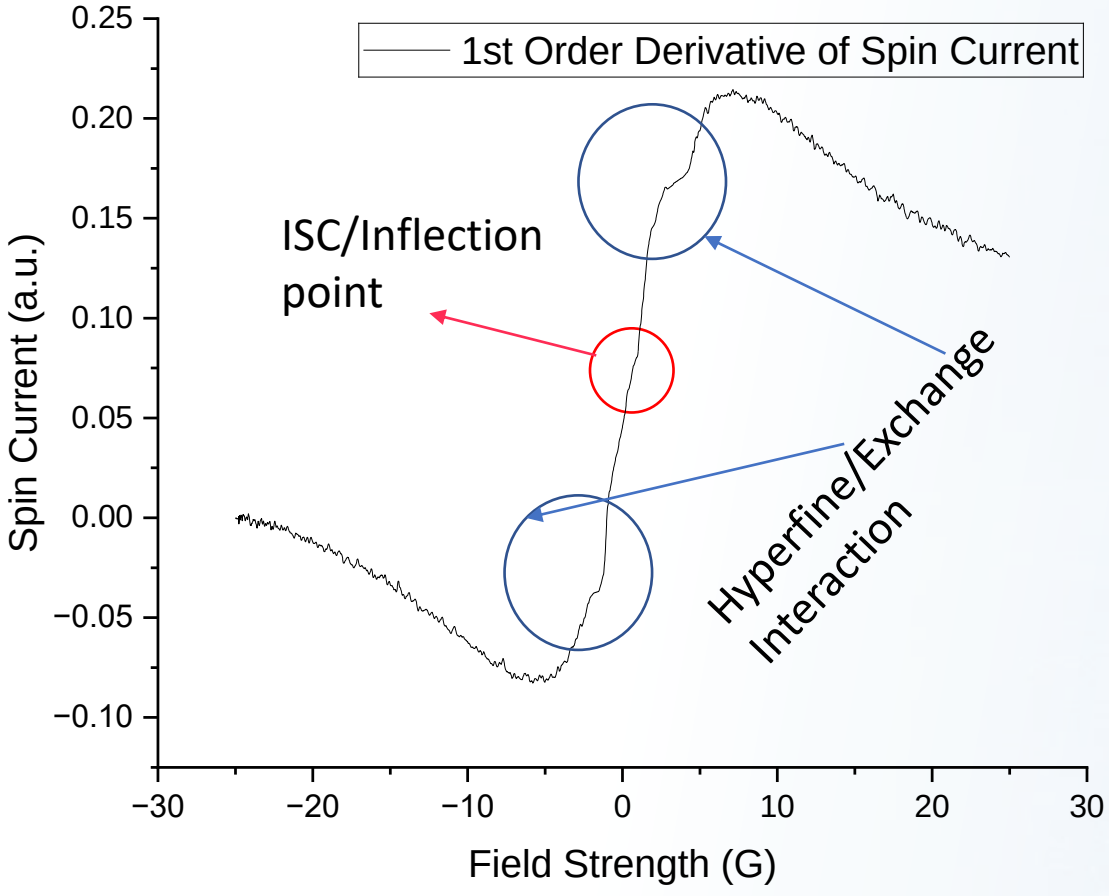
A.) 4 Volt Bias of 1st order derivative Identification of hyperfine and exchange interaction and singlet-triple mixing B.) 2nd order derivative 2.417 Gauss inflection point

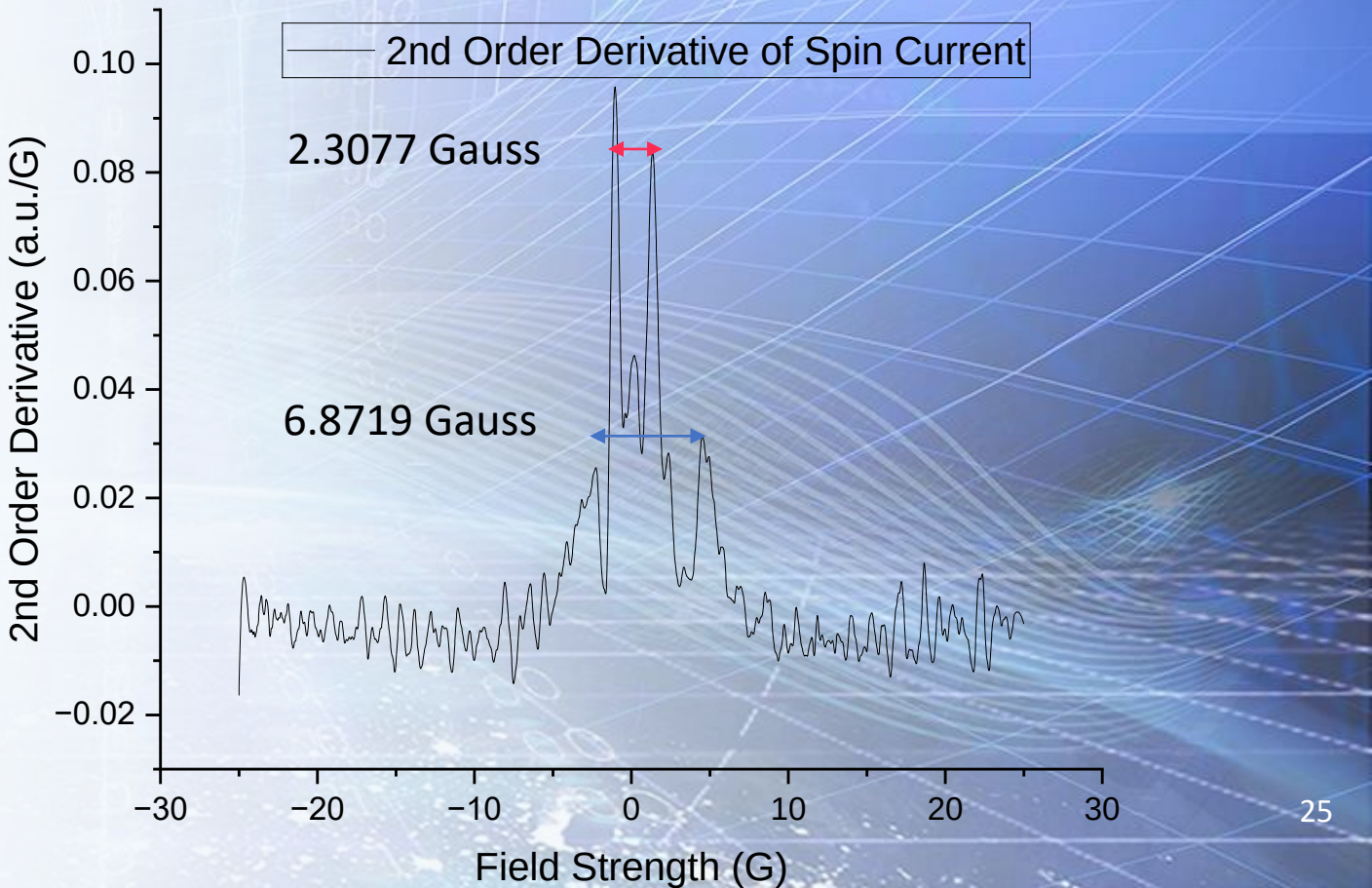
EDMR Spectra (4.5 Volt Bias)





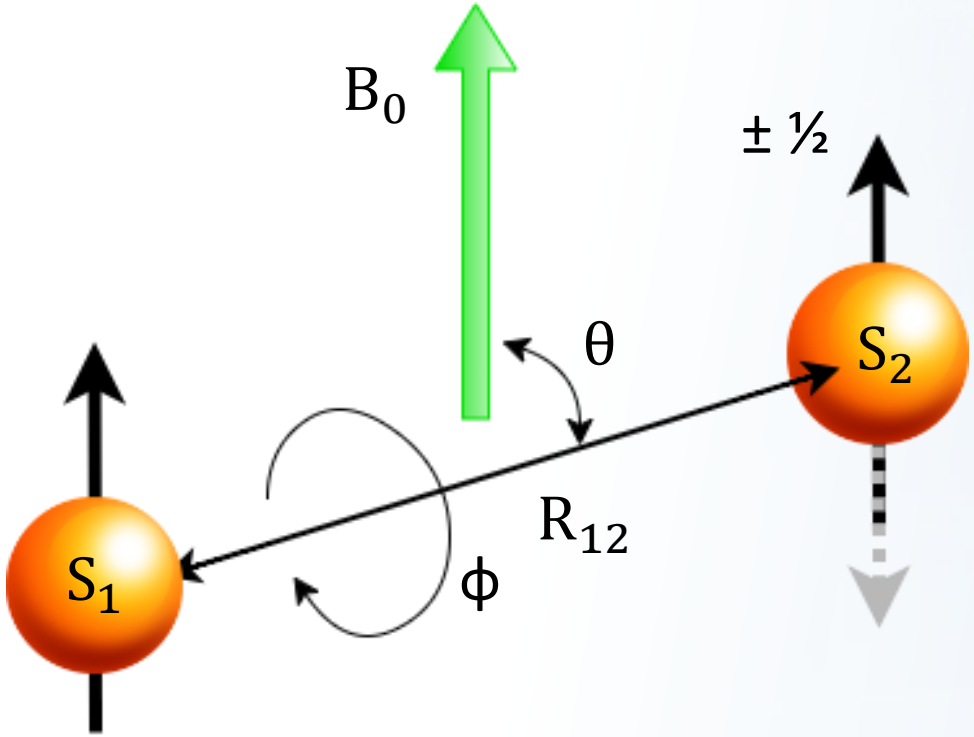
EDMR Spectra (5.0 Volt Bias)





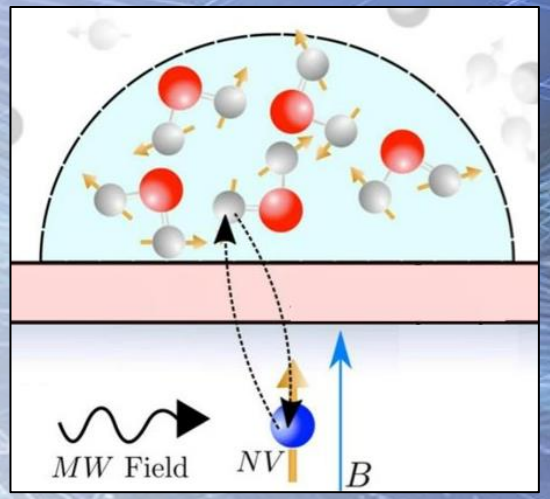
Future Research - *Potential Application*

Pulsed Electron DOuble Resonance (PELDOR) spectroscopy



- Observe dipole-dipole interaction between the spin defect in sensor and the electron spin in the material under test
- Achieve measurement for 10 ~ 20 nm distances
- Extrapolate the chemical environment around the electron

$$\omega_e = \frac{\mu_0}{4\pi\hbar}\frac{g_1 g_2 \mu_\beta}{r^3}(3\cos^2\theta - 1) = \omega_{dd}^0(3\cos^2\theta - 1)$$



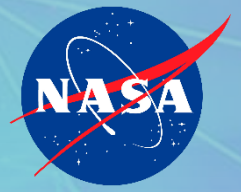
Conclusion

- The formation energy of the various types of defects in 6H-SiC was investigated. These findings are particularly important for studying the mechanism and process of EDMR spectroscopy on nitrogen/phosphorus implanted 6H-SiC devices. In future research, defect formation energy in 4H-SiC will be investigated particularly P substitutions and formed defects.

- The results seen thus far indicate a clear zero-field response, however, modulation frequency and amplitude still need optimization for further analysis. Additionally, the system is being upgraded to allow for an increased sweeping width of -125 G to 125 G which will allow for observation of full zero-field spectrum. Further testing on similar devices with different non-metal implants will soon be completed.

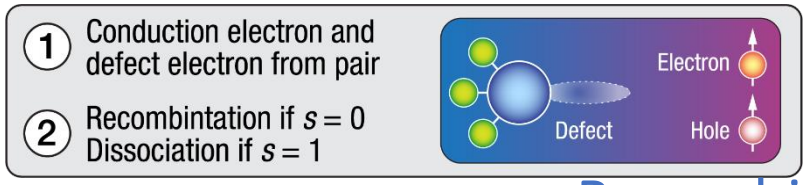
Acknowledgements

- I would like to thank NASA Glenn's Center Innovation Fund (CIF) for research assistance and financial support for the experimental effort toward this work, NASA Transformational, Technologies and Tools' (TTT) Innovative Measurements (IM) for supporting our time and attendance at this conference, and NASA Space Communications and Navigation (SCaN) for support of the interns and administrative tasks.
- Dr. Patrick Lenahan and team of Penn State
- Drs. Corey Cochrane and Hannes Kraus of JPL

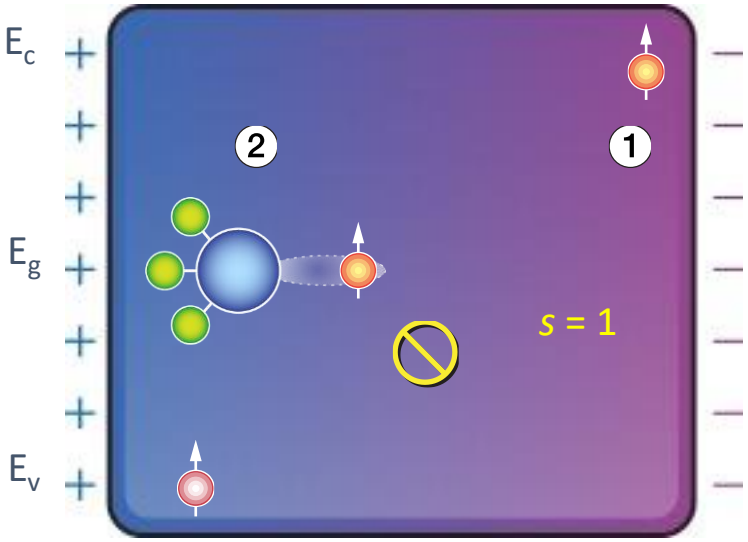


Questions?

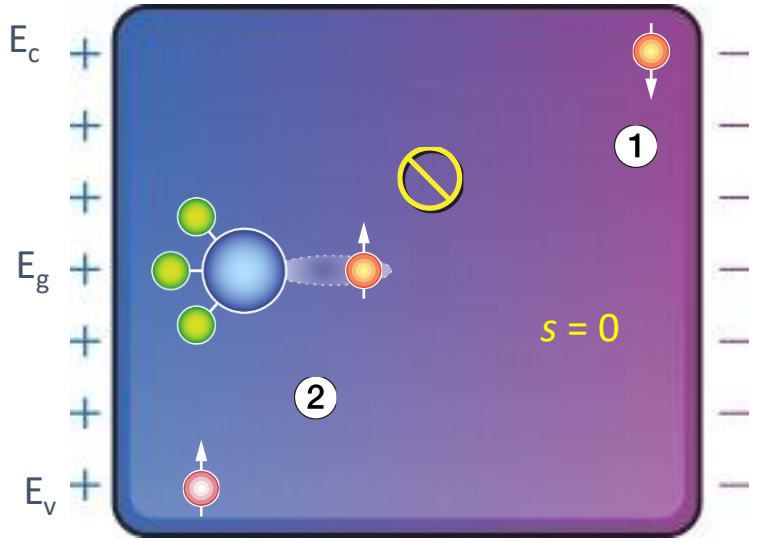
Spin-Dependent Recombination



Generation



Recombination



$$T_+ = \uparrow\uparrow$$
$$T_0 = (\uparrow\downarrow + \downarrow\uparrow)/\sqrt{2}$$
$$T_- = \downarrow\downarrow$$

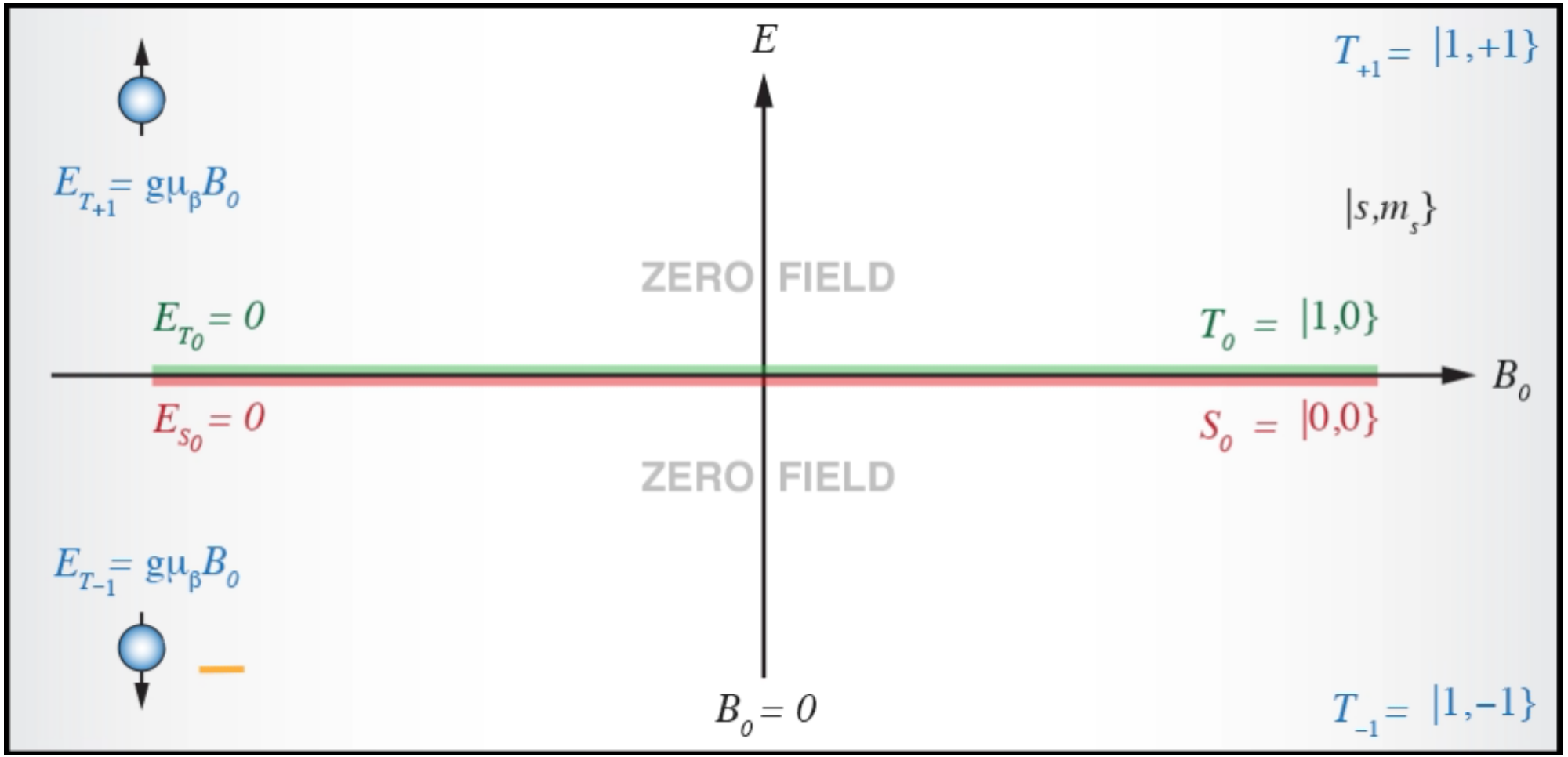
½ spin + ½ spin = 1

$$S_0 = (\uparrow\downarrow - \downarrow\uparrow)/\sqrt{2}$$

½ spin + ½ -hole spin = 0

Angular Momentum conserved

InterSystem Crossing and Degeneracy (ISC) (Electron Zeeman Interaction Only)



Dipole-Dipole Interaction

The energies are illustrated in the figure below. (D and E are denoted as D_1 and D_2, respectively.)

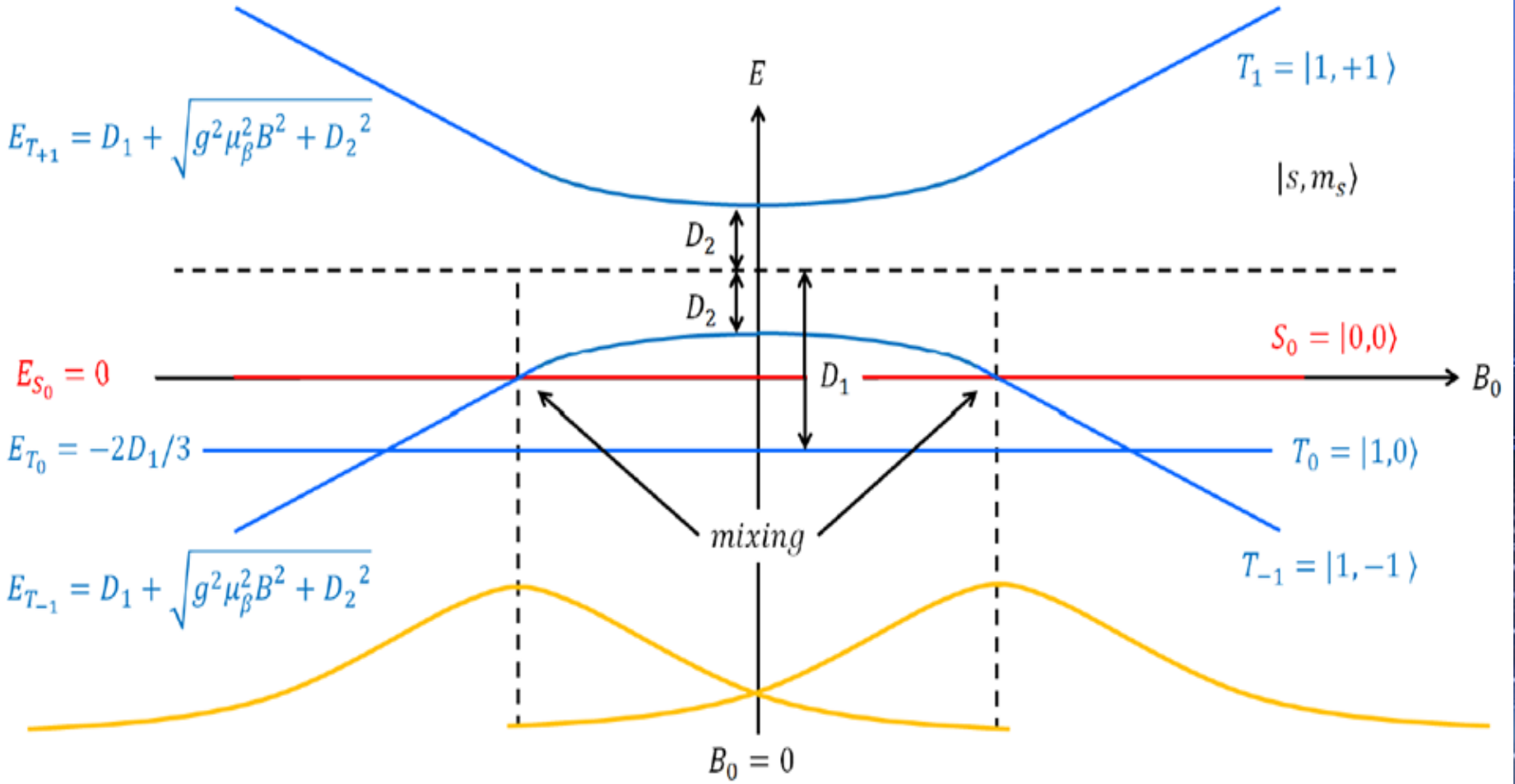
By using the two parameters D and E, and solving the Hamiltonian, one can get the allowed energies of the system.

$$E_{T_0} = -\frac{2}{3}D$$

$$E_{T_{+1}} = \frac{D}{3} + \sqrt{g^2\mu_\beta^2 B^2 + E^2}$$

$$E_{T_{-1}} = \frac{D}{3} - \sqrt{g^2\mu_\beta^2 B^2 + E^2}$$

$$E_{S_0} = 0$$



Exchange Interaction

Note that J_0 can be positive o negative, which means that the singlet can lie above or below the triplet states in energy. Typically, $J_0 > 0$ refers to ferromagnetic coupling, and $J_0 < 0$ refers to antiferromagnetic coupling.

The figure below illustrates the energies of the singlet and triplet states as a function of a magnetic field for $J_0 < 0$.